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APPLICATION NO.		FILING DATE	FIRST NAMED INVENTOR	ATTORNEY DOCKET NO.	CONFIRMATION NO.
09/644,937		08/23/2000	Anthony Nicholls	9476-003-999	1945
20583	7590	05/21/2002			
PENNIE A			EXAMINER		
1155 AVEN NEW YORK		THE AMERICAS 100362711		GALITSKY, NIKOLAI M	
				ART UNIT	PAPER NUMBER
				1631	7
				DATE MAILED: 05/21/2002	

Please find below and/or attached an Office communication concerning this application or proceeding.

		Applicant(s)				
. 0	9/644,937	NICHOLLS, ANTHONY				
Office Action Summary	xaminer	Art Unit				
Ni	ikolai M Galitsky	1631				
The MAILING DATE of this communication appears on the cover sheet with the correspondence address Period for Reply						
A SHORTENED STATUTORY PERIOD FOR REPLY IS SET TO EXPIRE 1 MONTH(S) FROM THE MAILING DATE OF THIS COMMUNICATION.  - Extensions of time may be available under the provisions of 37 CFR 1.136(a). In no event, however, may a reply be timely filed after SIX (6) MONTHS from the mailing date of this communication.  - If the period for reply specified above is less than thirty (30) days, a reply within the statutory minimum of thirty (30) days will be considered timely.  - If NO period for reply is specified above, the maximum statutory period will apply and will expire SIX (6) MONTHS from the mailing date of this communication.  - Failure to reply within the set or extended period for reply will, by statute, cause the application to become ABANDONED (35 U.S.C. § 133).  - Any reply received by the Office later than three months after the mailing date of this communication, even if timely filed, may reduce any earned patent term adjustment. See 37 CFR 1.704(b).  Status						
1) Responsive to communication(s) filed on						
	ction is non-final.					
3) Since this application is in condition for allowance except for formal matters, prosecution as to the merits is closed in accordance with the practice under <i>Ex parte Quayle</i> , 1935 C.D. 11, 453 O.G. 213.						
Disposition of Claims	, , , , , , , , , , , , , , , , , , , ,					
4) $\boxtimes$ Claim(s) <u>1-139</u> is/are pending in the application.						
4a) Of the above claim(s) is/are withdrawn from consideration.						
5) Claim(s) is/are allowed.						
6) Claim(s) is/are rejected.						
7) Claim(s) is/are objected to.						
8) Claim(s) 1-139 are subject to restriction and/or ele	ection requirement.					
Application Papers						
9) ☐ The specification is objected to by the Examiner.						
10) The drawing(s) filed on is/are: a) accepted	or b)  objected to by the Exa	aminer.				
Applicant may not request that any objection to the dra						
11) The proposed drawing correction filed on is:	a) approved b) disappr	oved by the Examiner.				
If approved, corrected drawings are required in reply to this Office action.						
12) The oath or declaration is objected to by the Examiner.						
Priority under 35 U.S.C. §§ 119 and 120						
13) Acknowledgment is made of a claim for foreign priority under 35 U.S.C. § 119(a)-(d) or (f).						
a) ☐ All b) ☐ Some * c) ☐ None of:						
<ol> <li>Certified copies of the priority documents had</li> </ol>	ave been received.					
<ol><li>Certified copies of the priority documents had</li></ol>	ave been received in Applicat	tion No				
<ul> <li>3. Copies of the certified copies of the priority documents have been received in this National Stage application from the International Bureau (PCT Rule 17.2(a)).</li> <li>* See the attached detailed Office action for a list of the certified copies not received.</li> </ul>						
14) Acknowledgment is made of a claim for domestic priority under 35 U.S.C. § 119(e) (to a provisional application).						
a) ☐ The translation of the foreign language provisional application has been received.  15)☐ Acknowledgment is made of a claim for domestic priority under 35 U.S.C. §§ 120 and/or 121.						
Attachment(s)						
1) Notice of References Cited (PTO-892) 2) Notice of Draftsperson's Patent Drawing Review (PTO-948) 3) Information Disclosure Statement(s) (PTO-1449) Paper No(s)	5) Notice of Informal	ry (PTO-413) Paper No(s) Patent Application (PTO-152)				

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## **DETAILED ACTION**

The art unit designated for this application has changed. Applicant(s) are hereby informed that future correspondence should be directed to Art Unit 1631.

## **Election/Restrictions**

Restriction to one of the following inventions is required under 35 U.S.C. 121:

- Group I Claims 1-21, drawn to a computer-implement method of finding an object in a group of N objects by minimal metric distance, classified in Class 702, subclass 27. If this Group is elected, than the below summarized sequence election is also required.
- Group II Claims 22-29, drawn to a method searching database of molecules for molecules that are similar to a target molecule by a method of determining a shape space of a set of molecules, classified in Class 707, subclass 100.

  If this Group is elected, than the below summarized sequence election is also required.
- Group III Claims 30-48, drawn to a mathematical method of constructing an ellipsoidal gaussian representation of a molecule field, classified in Class 703, subclass 2.
- Group IV Claims 49-56, drawn to a method of associating a first atom in a first molecule with an atom in a second molecule, classified in Class 703, subclass 12.

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Group V Claims 57-68, drawn to a method of searching database for at least one part of a molecule that is similar to at least one part of a target molecule structure, classified in Class 707, subclass 100.

Group VI Claims 69-78, drawn to a method of organizing a database via stored median, T, distances of N objects for facilitating searching the database, classified in Class 707, subclass 101. If this Group is elected, than the below summarized sequence election is also required.

Group VII Claims 79-96, drawn to a method of organizing database via minimal distance stored for K key objects in a database of N objects for facilitating searching the database, classified in Class 707, subclass 101. If this Group is elected, than the below summarized sequence election is also required.

Group VIII Claims 97-102, drawn to a mathematical method of constructing a pseudosurface of an ellipsoidal gaussian representations of a molecular field, classified in Class 703, subclass 2.

Group IX Claims 103-130, drawn to a method of constructing at least one single ellipsoidal gaussian function representation for a vacant space, classified in Class 703, subclass 2.

Group X Claims 131-136, drawn to a method of predicting the biological activity of a molecule of interest via statistical method, classified in Class 703, subclass 11.

Group XI Claim 137, drawn to a method of identifying a fragment of a molecule, classified in Class 702, subclass 29.

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Group XII Claims 138 and 139, drawn to a method of assessing the diversity of a set of molecules stored in a database on a computer, classified in Class 702, subclass 23.

The inventions are distinct, each from the other because of the following reasons:

The inventions of Groups I - XII are different inventions. The inventions of these Groups have different functions, different effects, and different modes of operation.

The invention of Group I is independent and distinct from those of Groups II, V-VII and XII because the method of finding, in group of N objects of Group I is directed to obtaining object by minimal metric distance, whereas in contrast Groups II, V-VII and XII are directed to store, organize and analyze a database via a shape space, store median, T, distances etc., for molecules that are similar to a target molecule, while being independent of the manner of obtaining said data which thus does not rely on, that is, is independent of or distinct from, the data supplied via Group I. The invention of Group II is directed to a computer-implement method of finding a subject, the invention of Group V is directed to a method of searching database, the invention of Group VII is directed to a method of organizing a database of N objects, the invention of Group VII is directed to a method of assessing the diversity of a set of molecules stored in a database. The inventions of these Groups have different functions, different effects, and different modes of operation.

The invention of Group I is independent and distinct from those of Groups III, VIII and IX because the method of finding, in group of N objects of Group I is directed to obtaining object by minimal metric distance, whereas in contrast Groups III, VIII and IX are directed to a

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method of constructing either an ellipsoidal gaussian representation of a molecule field or pseudo-surface, or vacant space. The inventions of these Groups have different effects.

The invention of Group I is independent and distinct from those of Groups IV and X-XI because the method of finding, in group of N objects of Group I is directed to obtaining object by minimal metric distance, whereas in contrast Groups IV and X-XI are directed to the methods of associating the atoms in a first and second molecules, predicting the biological activity and identifying a fragment of a molecule, respectively. The inventions of these Groups clearly have different functions, different effects, and different modes of operation.

The inventions of Groups II, V-VII and XII are independent and distinct from those of Groups III, VIII and IX because the method of the Groups II, V-VII and XII are directed to store, organize and analyze a database via a shape space, store median, T, distances etc., for molecules that are similar to a target molecule, whereas in contrast Groups III, VIII and IX are directed to a mathematical method of constructing either an ellipsoidal gaussian representation of a molecule field or pseudo-surface, or vacant space. The inventions of these Groups have different effects.

The inventions of Groups II, V-VII and XII are independent and distinct from those of Groups IV and X-XI because the method of the Groups II, V-VII and XII are directed to store, organize and analyze a database via a shape space, store median, T, distances etc., for molecules that are similar to a target molecule, whereas in contrast, contrast Groups IV and X-XI are directed to the methods of associating the atoms, predicting the biological activity and identifying a fragment of a molecule, respectively. The inventions of these Groups clearly have different functions, different effects, and different modes of operation.

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The inventions of Groups III, VIII and IX are directed to a mathematical method of constructing either an ellipsoidal gaussian representation of a molecule field or pseudo-surface, or vacant space, whereas in contrast, Groups IV and X-XI are directed to the methods of associating the atoms, predicting the biological activity and identifying a fragment of a molecule, respectively. The inventions of these Groups clearly have different functions, different effects, and different modes of operation.

## SPECIE ELECTION REQUIREMENT FOR GROUPS I, II AND VI, VII:

This application contains claim directed to the following patentably distinct species of the claimed invention: The species of Groups I, II and VI, VII are distinct because they each add a feature to the methods for finding an object, or determining a shape space, or organizing databases, with different and distinct functions; the species of these Groups are distinct from each other because they are independent, using a different type of the molecular fields, which each would require a separate and burdensome search, as defined above.

Groups I, II and VI, VII:

Specie A: a molecular field;

Specie B: steric field of a molecule;

Specie C: an electrostatic potential around a molecule;

Specie D; gaussian molecular field.

Applicant is required under 35 U.S.C. § 121 to elect a single disclosed species for prosecution on the merits to which the claims shall be restricted if no generic claim is finally held to be allowable. Currently, claims 1-3, 6, 14-18, 20 and 21 (Group I), claims 22 and 27-29

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(Group II), claims 69-73 and 78 (Group VI), and claims 79-85 and 91-95 (Group VII) are generic.

Applicant is advised that a response to this requirement must include an identification of the species that is elected consonant with this requirement, and a listing of all claims readable thereon, including any claims subsequently added. An argument that a claim is allowable or that all claims are generic is considered nonresponsive unless accompanied by an election.

Upon the allowance of a generic claim, applicant will be entitled to consideration of claims to additional species which are written in dependent form or otherwise include all the limitations of an allowed generic claim as provided by 37 C.F.R. § 1.141. If claims are added after the election, applicant must indicate which are readable upon the elected species. M.P.E.P. § 809.02(a).

Should applicant traverse on the ground that the species are not patentably distinct, applicant should submit evidence or identify such evidence now of record showing the species to be obvious variants or clearly admit on the record that this is the case. In either instance, if the examiner finds one of the inventions unpatentable over the prior art, the evidence or admission may be used in a rejection under 35 U.S.C. § 103 of the other invention.

Because these inventions are distinct for the reasons given above and have acquired a separate status in the art because of their recognized divergent subject matter, restriction for examination purposes as indicated is proper.

Applicant is advised that the response to this requirement to be complete must include an election of the invention to be examined even though the requirement be traversed (37 CFR § 1.143).

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Applicant is reminded that upon the cancellation of claims to a non-elected invention, the inventorship must be amended in compliance with 37 C.F.R. § 1.48(b) if one or more of the currently named inventors is no longer an inventor of at least one claim remaining in the application. Any amendment of inventorship must be accompanied by a diligently-filed petition under 37 C.F.R. § 1.48(b) and by the fee required under 37 C.F.R. § 1.17(h).

Papers related to this application may be submitted to Technical Center 1600 by facsimile transmission. Papers should be faxed to Technical Center 1600 via the PTO Fax Center located in Crystal Mall 1. The faxing of such papers must conform with the notices published in the Official Gazette, 1096 OG 30 (November 15, 1988), 1156 OG 61 (November 16, 1993), and 1157 OG 94 (December 28, 1993)(See 37 CFR § 1.6(d)). The CM1 Fax Center number is either (703) 308-4242 or (703) 305-3014.

Any inquiry concerning this communication or earlier communications from the examiner should be directed to Nikolai Galitsky, Ph.D., whose telephone number is (703) 308-2422. The examiner can normally be reached on Monday-Friday from 8:30 A.M. to 5 P.M.

If attempts to reach the examiner by telephone are unsuccessful, the examiner's supervisor, Michael Woodward, Ph.D., can be reached on (703) 308-4028.

Any inquiry of a general nature or relating to the status of this application should be directed to Patent Analyst, William Phillips, whose telephone number is (703) 305-3482 or to the Technical Center receptionist whose telephone number is (703) 308-0196.

May 18, 2002

NG

ARDIN H. MARSCHEL PRIMARY EXAMINER